PY2N20
Material Properties and Phase Diagrams
Lecture 1

P. Stamenov, PhD
School of Physics, TCD
Text Books

- *Materials Science & Engineering: An Introduction*
  William D *Callister*, Jr.
  S-LEN 620.11 53*5;1 .... 10

- *Introduction to Materials Science for Engineers*
  James F *Shackelford*
  620.11 M56*5
Handouts, Notes, Tutorials, etc.

- Handouts will be distributed at each of the lectures
- After the lectures electronic copies of the corresponding handouts will be uploaded at:
  http://physics.tcd.ie/people/Plamen.Stamenov/Courses/
- The examination questions are already fixed
- Voluntary tutorials to be organised...
Historical Perspective

- Metals, Polymers, Composites, Ceramics, Glasses

- Metals
  - Glassy metals
  - Al-lithium alloys
  - Dual phase steels
  - Microalloyed steels
  - New super alloys
  - Development slow: mostly quality control and processing

- Polymers, elastomers
  - High modulus polymers
  - Ceramic composites
  - Metal-matrix composites

- Composites
  - High temperature polymers
  - Titanium, Zirconium, Etc.
  - Alloys

- Ceramics, glasses
  - Refractories
  - Portland Cement
  - Fused Silica
  - Cements
  - Pyro-Ceramics
  - Tough engineering ceramics
  - (Al₂O₃, Si₃N₄, PSZ etc.)
Types of Materials

- Metals
- Ceramics
- Semiconductors
- Polymers
- Composites
Metals

Most elemental compounds are metals – rules of QM!
Ceramics

- Based on oxides, sulphides, nitrides, but not only!
Semiconductors

- Group IV (elemental), III-V’s, II-VI’s, others...
- Mainly organics, but not only...
What determines a material’s performance?

Properties ➔ Performance
Properties of Materials

- Mechanical
- Physical
  - Electrical
  - Thermal
  - Magnetic
  - Optical
  - Deteriorative
- Chemical
- Others
What determines a material’s performance?

Structure ➔ Properties ➔ Performance
What do we mean by structure?

- Macroscopic
- Microscopic
- Mesoscopic
- Nanoscopic
- Atomic level
Bonding

- Metallic Bonding
  - Conductivity
  - Ductility
  - Heat capacity
  - Reactivity
Bonding

- Covalent Bonding
  - Toughness
  - Brittleness
  - Insulation
  - Refractivity
  - Inactivity
Bonding

- Ionic Bonding
  - Brittleness
  - Insulation
  - Reactivity
Bonding

- Van der Waals Bonding
  - Weakness
  - Insulation
  - Inactivity
## Types of bonding in engineering materials

<table>
<thead>
<tr>
<th>Material Type</th>
<th>Bonding Character</th>
<th>Example</th>
</tr>
</thead>
<tbody>
<tr>
<td>Metal</td>
<td>Metallic</td>
<td>Iron, Cu</td>
</tr>
<tr>
<td>Ceramics and Glasses</td>
<td>Ionic/covalent</td>
<td>Silica (crystalline and amorphous)</td>
</tr>
<tr>
<td>Polymers</td>
<td>Covalent and secondary</td>
<td>Polyethylene</td>
</tr>
<tr>
<td>Semiconductors</td>
<td>Covalent or ionic/covalent</td>
<td>Si, CdS</td>
</tr>
</tbody>
</table>
Representation of Crystal Structures

- Atomic hard sphere model
- Packing density
- Lattices
- Unit cells
- Coordination spheres and polyhedra
- Point groups (of symmetry)
- Space groups
- ‘Colour’ groups
7 Crystal Systems
14 Crystal (Bravais) Lattices

CUBIC
\[ a = b = c \]
\[ \alpha = \beta = \gamma = 90^\circ \]

TETRAGONAL
\[ a = b \neq c \]
\[ \alpha = \beta = \gamma = 90^\circ \]

ORTHORHOMBIC
\[ a \neq b \neq c \]
\[ \alpha = \beta = \gamma = 90^\circ \]

HEXAGONAL
\[ a = b \neq c \]
\[ \alpha = \beta = 90^\circ \]
\[ \gamma = 120^\circ \]

MONOCLINIC
\[ a \neq b \neq c \]
\[ \alpha = \gamma = 90^\circ \]
\[ \beta \neq 120^\circ \]

TRICLINIC
\[ a \neq b \neq c \]
\[ \alpha \neq \beta \neq \gamma \neq 90^\circ \]

4 Types of Unit Cell
\[ P = \text{Primitive} \]
\[ I = \text{Body-Centred} \]
\[ F = \text{Face-Centred} \]
\[ C = \text{Side-Centred} \]

7 Crystal Classes → 14 Bravais Lattices
Atomic Packing Factor

\[ APF = \frac{\text{Volume of atoms in a unit cell}}{\text{Total volume of unit cell}} \]

**Homework**

Calculate the APF for

- (Primitive) cubic
  - BCC
  - FCC
Crytallographic Points, Directions and Planes

- Set up right-handed set of axes $x$, $y$, and $z$
  - $x$, $y$, and $z$ along the edges of a unit cell
  - Origin at a lattice point
  - $x$, $y$, and $z$ not always mutually perpendicular!
  - $a$, $b$, and $c$ are the unit length of the three corresponding unit cell edges

- Labelling conventions

<table>
<thead>
<tr>
<th>Points</th>
<th>Directions</th>
<th>Planes</th>
</tr>
</thead>
<tbody>
<tr>
<td>101</td>
<td>[110]</td>
<td>(110)</td>
</tr>
<tr>
<td>111</td>
<td>[111]</td>
<td>(100)</td>
</tr>
</tbody>
</table>

Families

- {001}
- <011>
What determines a material’s performance?

Basic aim of this short course

- Understand how processing affects the
  - Structure
  - Properties
  - Performance

of materials

- Concentrate (focus and emphasis) on metals, semiconductors, oxides...